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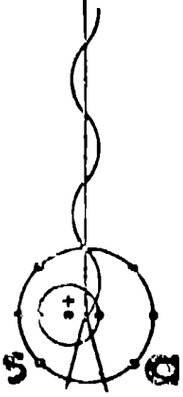

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AN APPROXIMATE INVERSION METHOD FOR FIVE POINT DIFFERENCE MATRIX EQUATIONS

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An Approximate Inversion Method (AIM) has been developed for solving two dimensional, five point difference matrix equations. The method is a variation of the Crout-Cholesky forward elimination and backward substitution method with operations on submatrix blocks rather than individual elements. A submatrix collapsing approximation makes the method efficient; applying familiar element operations on submatrix blocks makes it simple. Global and line rebalance are used to define an optimum relaxation parameter to accelerate convergence of the iterative algorithm.

AIM is compared with the Successive Line OverRelaxation (SLOR) and Strongly Implicit Procedure (SIP) methods in a numerical study. These methods were applied to solving the fluid dynamics and neutron diffusion equations. AIM was found to be 1.3 to 2.5 times faster than SIP and 1.8 to 5.4 times faster than SLOR. Rebalance relaxation enhanced AIM stability over that of the other methods.

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AN APPROXIMATE INVERSION METHOD FOR FIVE POINT DIFFERENCE MATRIX EQUATIONS

INTRODUCTION

SIMMER,[1] a best estimate computer program for LMFBR disrupted core analysis, is being developed at the Los Alamos Scientific Laboratory. Recent fluid dynamics methods development for SIMMER was concerned with enhancing numerical stability and reducing calculational effort. One such development considered the evaluation of the pressure change and material density change distributions during a time step. The spatially uncoupled approximate solution to be iterated was replaced with a correct spatially coupled simultaneous solution. This resulted in decreased calculational effort per time step as well as enhanced stability to allow much larger time steps to be taken. This improvement was realized by formulating the correct five diagonal matrix equations in two dimensional rectilinear geometry and then solving them with an efficient matrix inversion routine. Initially, the Successive Line OverRelaxation (SLOR)[2,3] method was used to solve these matrix equations. Instances of weakly diagonally dominant matrices requiring hundreds of SLOR iterations to invert them prompted consideration of a more efficient method.

A new Approximate Inversion Method (AIM) was felt to have this efficiency. The method is a variation of the direct Crout-Cholesky forward elimination and backward substitute method.[2] Crout-Cholesky method element operations on a tridiagonal element matrix are applied in AIM as submatrix block operations on a tridiagonal block matrix. To make the method efficient, a submatrix collapsing approximation is applied. Making this approximation requires that the method be iterative. A description of this iterative algorithm and its approximate matrix inversion follows.

METHOD

ITERATIVE ALGORITHM

The matrix equation to be solved is

$$\underline{\underline{M}} \cdot \underline{F} = \underline{Q} \qquad (1)$$

where

$\underline{\underline{M}}$ is a known five diagonal element irreducible M matrix[3] with tridiagonal submatrix blocks such that $\underline{\underline{M}} = \underline{\underline{L}} + \underline{\underline{D}} + \underline{\underline{U}}$, $\underline{\underline{D}}$ is a block diagonal matrix with tridiagonal element submatrices and $\underline{\underline{L}}$ and $\underline{\underline{U}}$ are adjacent lower and upper block diagonal matrices, respectively, with diagonal element submatrices;

$\underline{Q}$ is a known vector; and

$\underline{F}$ is an unknown vector to be determined.

To evaluate the solution, AIM requires an n=0 iteration initial estimate of $\underline{F}$, $\underline{F}^0$. The error in $\underline{Q}$ corresponding to the n^{th} iteration estimate of $\underline{F}$ is

$$\underline{\Delta Q}^n = \underline{Q} - \underline{\underline{M}} \cdot \underline{F}^n \quad . \tag{2}$$

The change in $\underline{F}^n$ needed to remove this error can be determined by solving the matrix equation

$$\underline{\underline{M}} \cdot \underline{\Delta F}^n = \underline{\Delta Q}^n \quad . \tag{3}$$

An approximate inversion of $\underline{\underline{M}}$, however, gives only an approximate solution,

$$\underline{\Delta F}^n \cong (\underline{\underline{M}}^{approximate})^{-1} \cdot \underline{\Delta Q}^n \quad . \tag{4}$$

Because $\underline{\Delta F}^n$ is approximate, combining it with $\underline{F}^n$ defines only the next iteration estimate of $\underline{F}$, i.e., $\underline{F}^{n+1}$. To accelerate convergence of $\underline{F}^{n+1}$ to $\underline{F}$, a diagonal element relaxation matrix $\underline{\underline{W}}$ is applied to $\underline{\Delta F}^n$,

$$\underline{F}^{n+1} = \underline{F}^n + \underline{\underline{W}} \cdot \underline{\Delta F}^n \quad . \tag{5}$$

Three definitions of $\underline{\underline{W}}$ have been considered:

1. $w_{\ell\ell} = 1$, no relaxation;
2. $w_{\ell\ell} = w$, global rebalance relaxation; and
3. $w_{\ell\ell} = w_j$, line rebalance relaxation where $j = 1 + (\ell-1)/I$ and I is the number of nodes in a line.

The w and w_j rebalance parameters are defined to minimize the remaining Euclidean norm error in $\underline{Q}$.

$$\begin{aligned} \text{Error} &= (\underline{\Delta Q}^{n+1}, \underline{\Delta Q}^{n+1}) \\ &= \sum_{\ell}^{[*J} (\Delta Q_\ell^{n+1})^2 \\ &= \sum_{\ell}^{[*J} (\Delta Q_\ell^n - w_{\ell\ell}\, \Delta^2 Q_\ell^n)^2 \end{aligned} \tag{6}$$

where

$$\underline{\Delta^2 Q}^n = \underline{\underline{M}} \cdot \underline{\Delta F}^n \quad .$$

Error is minimized with respect to w or w_j by requiring dError/dw = 0 or ∂Error/∂w_j = 0 for j=1,2...,J, respectively. The dError/dw = 0 requirement can be solved for w giving

$$w = \frac{\sum_{\ell}^{I*J} \Delta Q_{\ell}^{n} \, \Delta^2 Q_{\ell}^{n}}{\sum_{\ell}^{I*J} (\Delta^2 Q_{\ell}^{n})^2} \quad . \tag{7}$$

The ∂Error/∂w_j = 0 requirement of J equations gives a five diagonal element matrix equation with spatial coupling to the four nearest node lines. This matrix equation is solved for w_j, j=1,2,...J, by forward elimination of the two lower diagonals and backward substitution into the two modified upper diagonals. Having relaxed $\underline{F}^{n+1}$ by one of the above definitions of $\underline{\underline{W}}$, the iterative evaluation continues until the convergence criterion

$$\frac{(\underline{\Delta Q}^{n+1}, \underline{\Delta Q}^{n+1})}{(\underline{Q}, \underline{Q})} < \varepsilon \, , \tag{8}$$

is satisfied for some small ε.

MATRIX INVERSION

The block tridiagonal matrix $\underline{\underline{M}}=\underline{\underline{L}}+\underline{\underline{D}}+\underline{\underline{U}}$ is inverted by forward eliminating its lower block diagonal $\underline{\underline{L}}$ and backward substituting into its modified upper block diagonal $\underline{\underline{U}}^*$. The procedure for forward eliminating $\underline{\underline{L}}$ involves stepping along the j=1,2,...J-1 node lines and eliminating the $(j+1)^{th}$ node line submatrix $\underline{\underline{L}}_{j+1}$. One starts by setting

$$\underline{\underline{D}}_1^* = \underline{\underline{D}}_1 \tag{9}$$

and

$$\underline{\Delta Q}_1^{+n} = \underline{\Delta Q}_1^{n} \tag{10}$$

for the first node line. Then for each j^{th} node line, starting with j = 1, the tridiagonal element submatrix $\underline{\underline{D}}_j^*$ is directly inverted by the Crout-Cholesky forward elimination and backward substitution method. $\underline{\underline{U}}_j$ becomes $(\underline{\underline{D}}_j^*)^{-1} \cdot \underline{\underline{U}}_j$, a full element submatrix, and $\underline{\Delta Q}_j^{+n}$ becomes

$$\underline{\Delta Q}_j^{*n} = (\underline{\underline{D}}_j^*)^{-1} \cdot \underline{\Delta Q}_j^{+n} \quad . \tag{11}$$

An elementwise collapsing approximation is now made on the full submatrix $(\underline{\underline{D}}_j^*)^{-1} \cdot \underline{\underline{U}}_j$. Row elements to the left and right of the submatrix diagonal element are collapsed (summed) to the adjacent left and right elements, respectively,

$$\underline{\underline{U}}_j^* \xleftarrow[\text{approximation}]{\text{collapse}} (\underline{\underline{D}}_j^*)^{-1} \cdot \underline{\underline{U}}_j \quad . \tag{12}$$

$(\underline{\underline{D}}_j^*)^{-1} \cdot \underline{\underline{U}}_j$ becomes the tridiagonal element submatrix $\underline{\underline{U}}_j^*$.

Thus far, our purpose has been to convert the tridiagonal submatrix $\underline{\underline{D}}_j^*$ to an identity submatrix. $\underline{\underline{L}}_{j+1}$ can now be eliminated from the $(j+1)^{th}$ row submatrix equation by multiplying the modified j^{th} row submatrix equation by the diagonal element submatrix $\underline{\underline{L}}_{j+1}$ and then subtracting it from the $(j+1)^{th}$ row equation giving

$$\underline{\underline{D}}_{j+1}^* = \underline{\underline{D}}_{j+1} - \underline{\underline{L}}_{j+1} \cdot \underline{\underline{U}}_j^* \quad \text{and} \tag{13}$$

$$\underline{\Delta Q}_{j+1}^{+n} = \underline{\Delta Q}_{j+1}^{n} - \underline{\underline{L}}_{j+1} \cdot \underline{\Delta Q}_j^{*n} \quad . \tag{14}$$

At this point, the reason for collapsing $(\underline{\underline{D}}_j^*)^{-1} \cdot \underline{\underline{U}}_j$ to the tridiagonal element submatrix $\underline{\underline{U}}_j^*$ becomes evident. The tridiagonal element form of $\underline{\underline{D}}_{j+1}$ is maintained during its modification to $\underline{\underline{D}}_{j+1}^*$. Without the collapsing approximation, $\underline{\underline{D}}_{j+1}^*$ would be a full element submatrix. Inverting $\underline{\underline{D}}_{j+1}^*$ in the next step can now be done efficiently by the Crout-Cholesky method rather than by a full element submatrix inversion.

After stepping forward with the above procedure for each j=1,2,...,J-1 line, the solution estimate in the J^{th} (last) node line is determined by

$$\underline{\Delta F}_J^n = (\underline{\underline{D}}_J^*)^{-1} \cdot \underline{\Delta Q}_J^{+n} \quad . \tag{15}$$

At this point, $\underline{\underline{L}}$ has been eliminated, $\underline{\underline{D}}$ has become the identity matrix $\underline{\underline{I}}$, and $\underline{\underline{U}}$ has been modified to $\underline{\underline{U}}^*$ having tridiagonal element submatrix blocks. To complete the solution, backwards substitute into the $\underline{\underline{I}} + \underline{\underline{U}}^*$ upper triangular matrix to determine

$$\underline{\Delta F}_j^n = \underline{\Delta Q}_j^{*n} - \underline{\underline{U}}_j^* \cdot \underline{\Delta F}_{j+1}^n \qquad \text{for } j=J-1,J-2,\ldots,1 \quad . \tag{16}$$

The variable storage for AIM is approximately twice that of SLOR. The original matrix equation must be saved to evaluate Equation (2) each iteration. In addition, $\underline{\Delta Q}^n$, $\underline{\underline{D}}_j^*$ and $\underline{\underline{U}}_j^*$ for j=1,2,...J, and the line rebalance matrix equation must be assigned storage. The 7*I*J storage locations of the original matrix equation expand to 14*I*J + 7*J locations to evaluate the solution. The fact that $\underline{\underline{D}}_j^*$ and $\underline{\underline{U}}_j^*$ for j=1,2,...J are evaluated and saved in the first iteration eliminates the need to reevaluate them in subsequent iterations. Only Equations (11) and (14)-(16) need to be evaluated in subsequent iterations. This reduces the calculational effort per iteration by 40%.

Applying AIM with no relaxation on a strongly coupled, weakly diagonally dominant matrix equation can result in a divergent algorithm. Two examples of this will be discussed in the numerical study section. This occurs when the approximation of $\underline{\underline{M}}$ during its inversion causes it to lose diagonal dominance. Divergence can be prevented in two ways. The approximation of $\underline{\underline{M}}$ during its inversion can be constrained to maintain diagonal dominance through further modification. Another way is to use rebalance relaxation when AIM with no relaxation is found to diverge. This latter approach is recommended because divergence of AIM with no relaxation occurs when $\underline{\underline{M}}$ is weakly diagonally dominant, a situation where rebalance relaxation would be more efficient. The stablizing effect of rebalance relaxation has been found to override any instability due to modifying $\underline{\underline{M}}$ during its inversion.

NUMERICAL STUDY

FLUID DYNAMICS

This developmental effort has resulted in AIM and SLOR being programmed in the SIMMER-II fluid dynamics algorithm. Their relative efficiency can now be compared in this convenient framework. The transition phase and work energy test problems in the SIMMER-II manual[1] were used for this comparison. Can wall restraint on radial motion was removed in both problems inorder to have two dimensional spatial coupling. Selecting these problems was based on their availability and small computing requirement. Their coarse spatial mesh, however, means that both methods converge rapidly. Problems with stronger spatial coupling would be of interest. A comparison for such a problem will also be given.

The number of iterations and calculation times of AIM and SLOR were monitored when evaluating the two test problems. SLOR required four times as many iterations and twice the calculational effort of AIM with no relaxation to solve the pressure change matrix equation. Equal computation times were required for the material density matrix equations because SLOR converged in two iterations and AIM converged in one iteration. The SLOR solutions were evaluated by beginning with no relaxation and then updating the relaxation parameter every five iterations based on the last iteration error ratio. Applying global and line rebalance relaxation in AIM increased calculational effort per iteration by 20% and 30%, respectively. For these small test problems, AIM with no rebalance relaxation was more efficient. However, for large problems with strong spatial coupling, the rebalance options would become more efficient. This occurs when their ability to enhance convergence and reduce the number of iterations overcomes their additional calculational effort per iteration.

An example of how effective rebalance relaxation can be was obtained from a realistic 16 by 31 mesh transition phase analysis problem[4] run on SIMMER-II. Liquid fuel was in the process of entering the coolant channel with large local FCI pressure spikes occurring. The SIMMER-II run aborted when the pressure change solution evaluated by AIM with no relaxation diverged. This was caused by the loss of diagonal dominance through modifying M during its inversion. Restarting SIMMER-II using the SLOR method resulted in several hundred iterations to obtain a converged solution. Restarting SIMMER-II using the AIM method with global rebalance relaxation, however, required fewer than ten iterations to converge the pressure change solution.

NEUTRON DIFFUSION

It became of interest, after finding AIM to be faster than SLOR for the fluid dynamics equations, to compare AIM with the Strongly Implicit Procedure (SIP) method.[5] The existence of a few group, two dimensional neutron diffusion equation program[6] employing the SIP method provided a convenient framework for such a comparison. Making the comparison involved replacing the SIP method subroutine in the diffusion program with the AIM and SLOR subroutines from SIMMER-II. The two energy group IAEA LWR benchmark problem[7] and the four energy group SNR-300 LMFBR benchmark problem[8] were then evaluated by the diffusion equation program using each method. The LWR quarter core configuration was evaluated with a 44 by 44 mesh having a 4 cm mesh size. The LMFBR quarter core configuration was evaluated with a 34 by 34 mesh having a 2.7 cm mesh size. The methods were compared during outer iteration 3 inorder to reduce the effect of the initial few group flux guess.

The convergence behavior of each method in each energy group of the LWR problem is shown in Figures 1-2. Several SIP solutions with different acceleration parameter values are shown. The optimally accelerated SIP solution can be seen among them. The SLOR solution was evaluated with relaxation parameter updates every five iterations. AIM with no relaxation was found to be the fastest method for this problem. For practical error reduction levels of two to six decades, AIM was faster than SIP by factors of 1.3 to 1.6 and faster than SLOR by factors of 1.8 to 3.0. In a comparison of calculational effort per iteration to that of AIM with no relaxation, SLOR required 41% less, SIP required 22% more, AIM with global rebalance required 32% more, and AIM with line rebalance required 30% more. The comparison of AIM and SLOR in this problem is similar to what was observed in the fluid dynamics test problems.

The convergence behavior of each method in each energy group of the LMFBR problem is shown in Figures 3-6. Calculations similar to those in the LWR problem were performed. Because of stronger spatial coupling in this problem, the convergence rate of AIM with no relaxation deteriorated relative to the other methods. The possibility for divergence, spoken of earlier, is seen to occur in energy group 2. Note, however, that during the first few iterations AIM with no relaxation converged as fast as the best method, AIM with global or line rebalance relaxation. For practical error reduction levels of two to six decades, AIM with rebalance relaxation was found to be faster than optimum SIP by factors of 1.4 to 2.5 and faster than SLOR by factors of 3.0 to 5.4. In a comparison of calculational effort per iteration to that of AIM with no relaxation, SLOR required 44% less, SIP required 31% more, AIM with global rebalance required 29% more, and AIM with line rebalance required 35% more.

It should be mentioned that SIP experienced several instances of convergence to error reduction levels of 10^{-3} to 10^{-5} followed by subsequent oscillation about that level. This occurred in outer iterations 1 and 2 for acceleration parameters greater than 0.9. For these same acceleration parameter values, an oscillating convergence rate can be seen in Figures 5-6 for energy groups 3 and 4 in outer iteration 3.

CONCLUSIONS

A new Approximate Inversion Method (AIM) has been developed for solving two dimensional, five point difference matrix equations. Familiar Crout-Cholesky method element operations applied to submatrix blocks makes the method simple. A submatrix collapsing approximation and iterative acceleration by rebalance relaxation make the method efficient.

A numerical study comparing AIM to the Successive Line OverRelaxation (SLOR) and Strongly Implicit Procedure (SIP) methods has shown AIM to be superior. This comparison was made by solving the fluid dynamics and neutron diffusion equations. AIM with no relaxation acceleration was fastest for problems with weak spatial coupling. On the other hand, AIM with global or line rebalance relaxation was fastest for problems with strong spatial coupling. The best strategy for AIM appears to be the use of no relaxation during the initial iterations and then switching to rebalance relaxation when the convergence rate with no relaxation starts to deteriorate.

The efficiency of SIP could be improved to the level of AIM for problems with strong spatial coupling by applying global or line rebalance relaxation in SIP. To achieve this level of efficiency, however, requires that a good estimate for the SIP acceleration parameter be known apriori. Too large a value causes oscillations; too small a value slows convergence. Not having to select such an acceleration parameter makes AIM a more attractive method.

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Figure 1. Error Versus Time for the LWR Problem, Energy Group 1

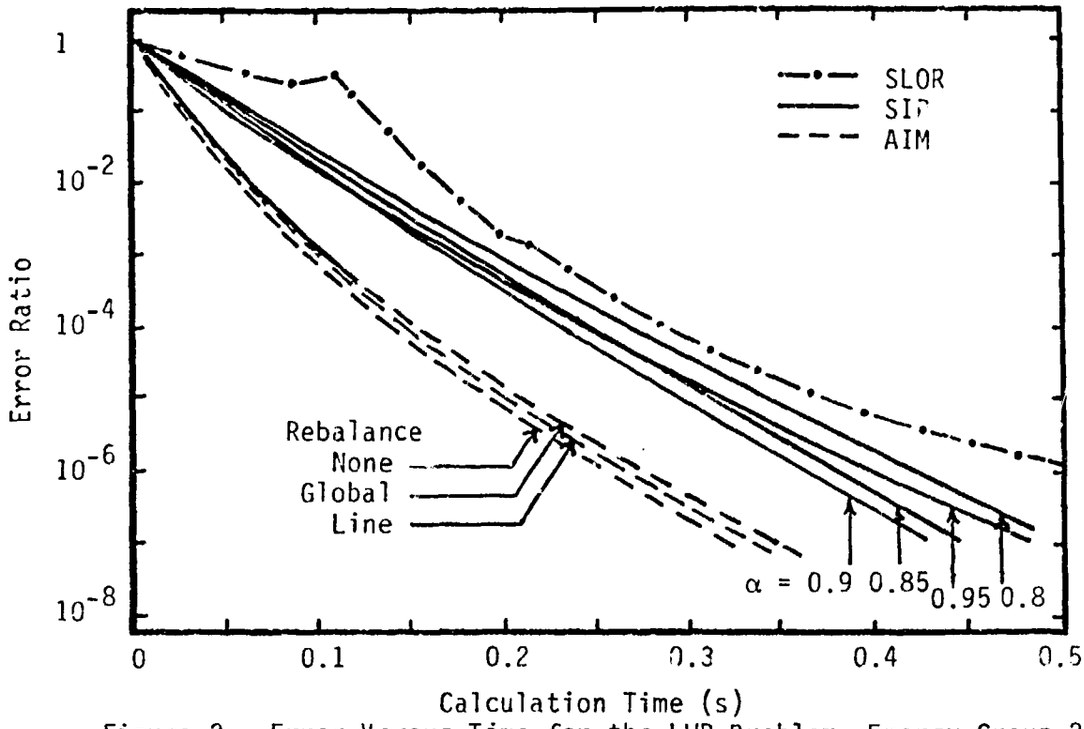

Figure 2. Error Versus Time for the LWR Problem, Energy Group 2

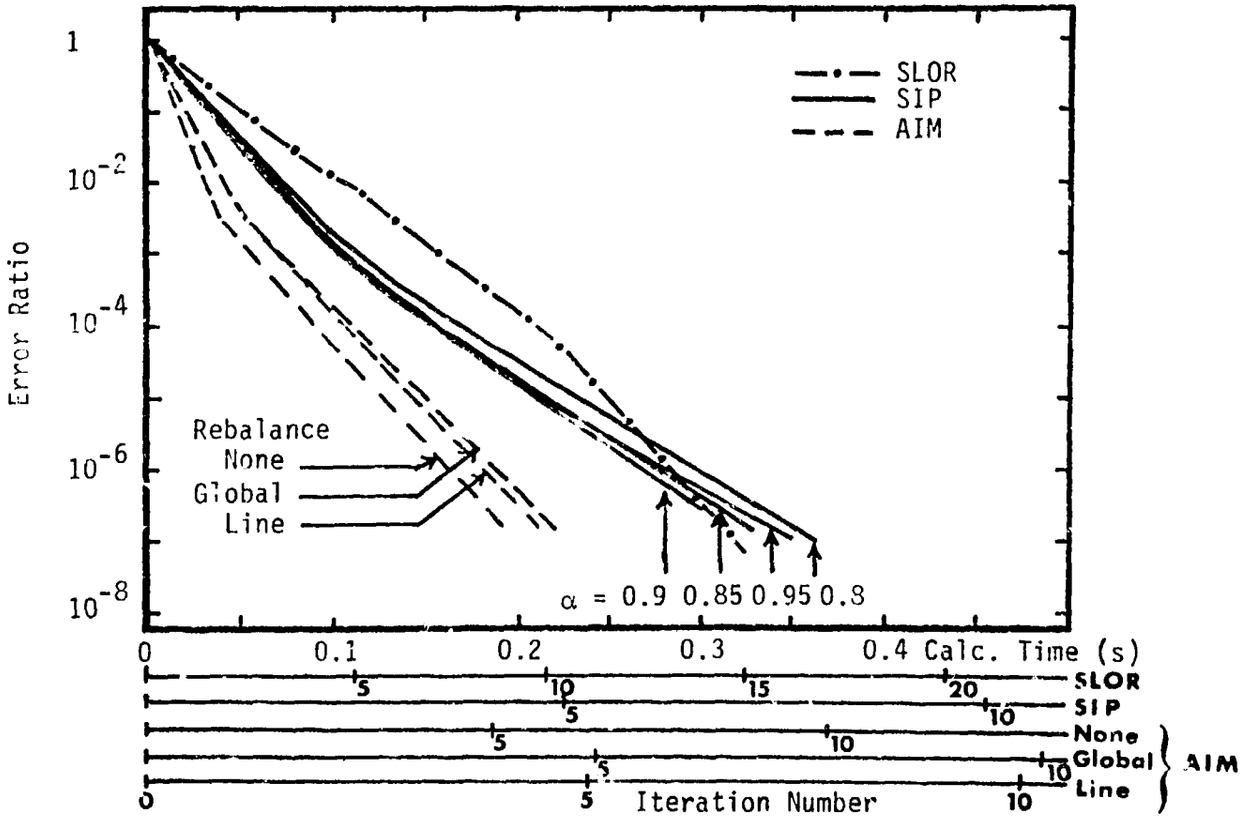

Figure 3. Error Versus Time for the LMFBR Problem, Energy Group 1

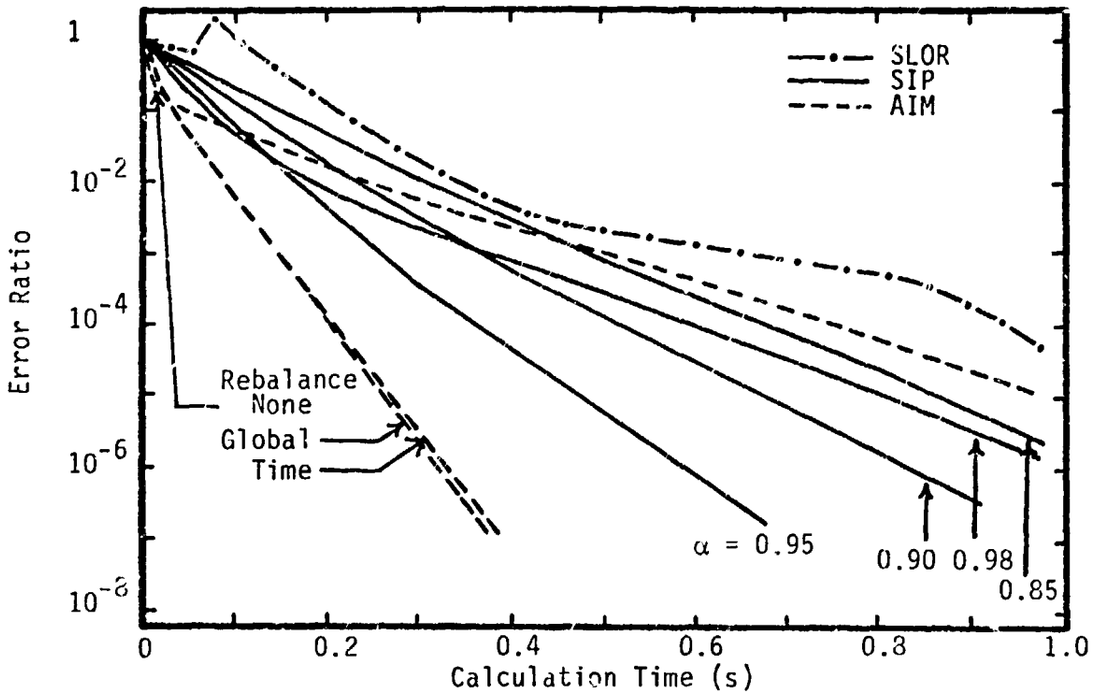

Figure 4. Error Versus Time for the LMFBR Problem, Energy Group 2

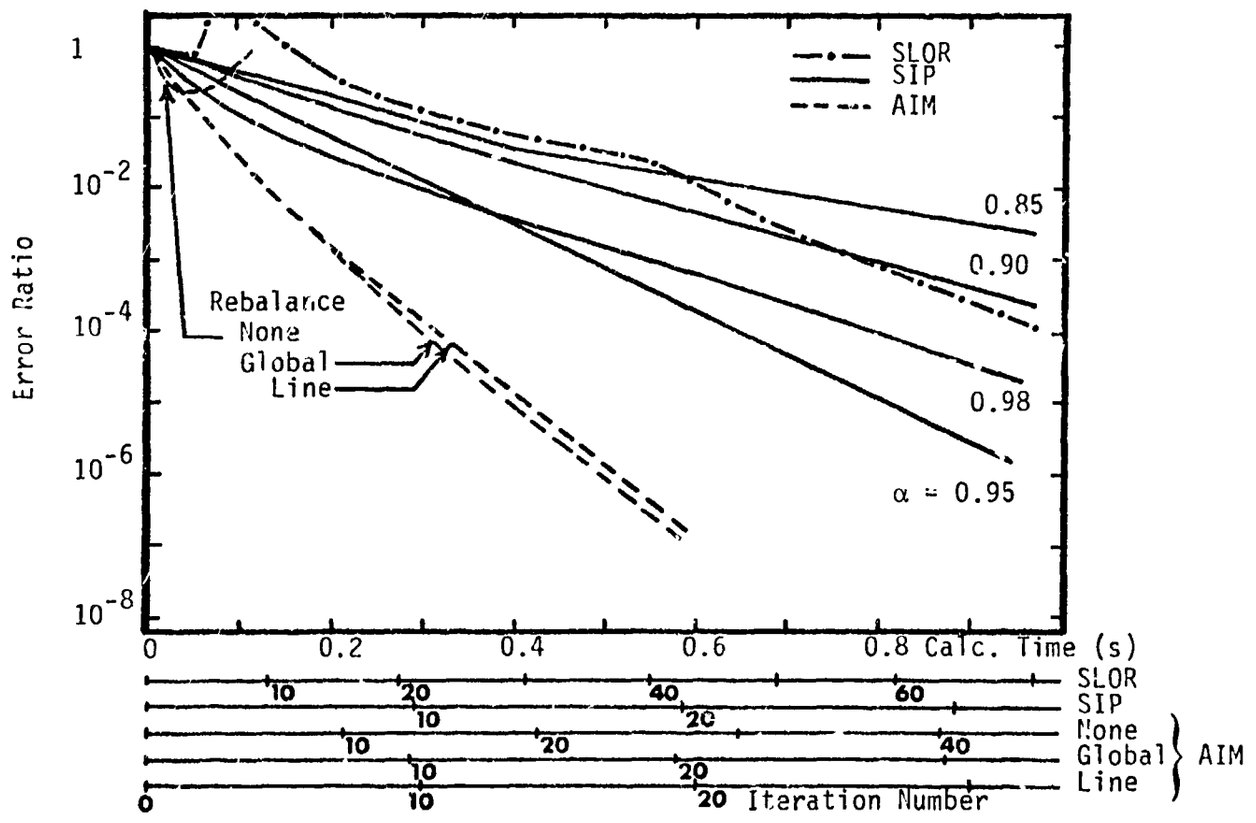

Figure 5. Error Versus Time for the LMFBR Problem, Energy Group 3

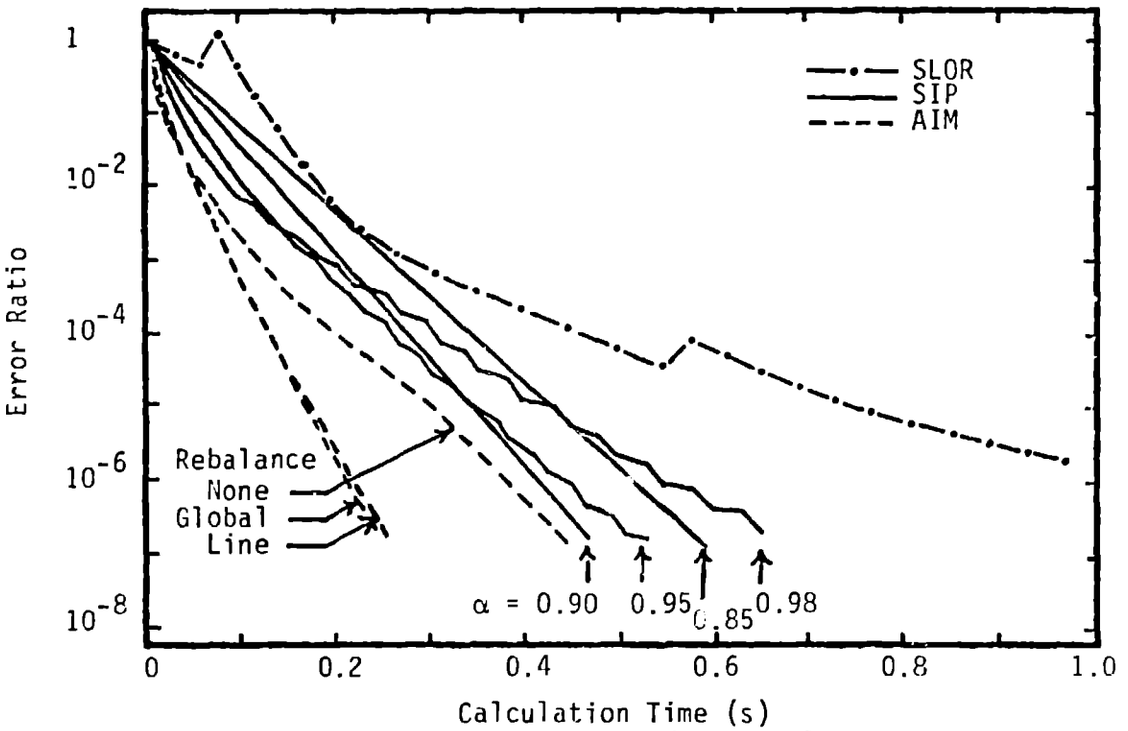

Figure 6. Error Versus Time for the LMFBR Problem, Energy Group 4